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Correlated ab initio methods for the description of RIXS excitations in solids

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Fully ab initio wavefunction-based methods from modern quantum chemistry are employed for the study of the electronic structure of correlated transition-metal com- pounds. We focus on the computation of N-particle excitations like those probed by optical absorption or RIXS (resonant inelastic x-ray scattering) measurements. The strong correlations are treated within the CASSCF (complete-active-space self- consistent-field) approximation while remaining correlation effects are handled by either multireference configuration-interaction techniques or second-order perturba- tion theory [1]. Since such correlation calculations can be carried out only for a finite region of the extended crystal, the remaining part of the solid is described at the Hartree-Fock level [2]. Results for the d-orbital electronic structure and su- perexchange interactions in a number of layered Cu and Ir oxide compounds are compared with recent RIXS data.

[1] T. Helgaker, P. Jørgensen, and J. Olsen, Molecular Electronic-Structure Theory (Wiley, Chichester, 2000)
[2] L. Hozoi, L. Siurakshina, P. Fulde, and J. van den Brink, Nature Sci. Rep., in press (available at arXiv:1012.3603)

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Talk

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